

Methanol
67-56-1 | DTXSID2021731

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 69.1 °C

Global applicability domain: Outside

Local applicability domain index: 3.65e-01

Confidence level: 7.55e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Methanol</div> <div>Measured: 64.7</div> <div>Predicted: 69.1</div>	<div>Image not found</div> <div>Ethanol</div> <div>Measured: 78.2</div> <div>Predicted: 80.5</div>	<div>Image not found</div> <div>Ethyl hydroperoxide</div> <div>Measured: 95.0</div> <div>Predicted: 99.9</div>
<div>Image not found</div> <div>Isopropanol</div> <div>Measured: 82.3</div> <div>Predicted: 90.0</div>	<div>Image not found</div> <div>1-Propanol</div> <div>Measured: 97.2</div> <div>Predicted: 96.5</div>	